

FORMATION OF JUNCTIONS AND DEFECTS IN CARBON NANOTUBES

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Abstract

Future generation of electronic devices made by carbon nanotubes may critically depend on how the junctions between different nanotubes can be manufactured. Thin single-walled carbon nanotubes (SWNTs) could be welded together by heating to form molecular multiterminal junctions at elevated temperature without initially introducing structural defects such as vacancies and interstitials. This was demonstrated by classical molecular dynamics calculations with empirical Brenner potential to simulate the dynamic formation pathway of junctions between crossing nanotube pairs. Junctions are established through forming new intertube sp^3 -like covalent bonds, followed by breaking up bonds in the original nanotubes. The final configuration of junctions depends on the diameter of SWNTs, chirality of the crossing tube pairs, initial intertube distance and temperature. The size of SWNTs also affects the minimum temperature for junction formation. The larger the diameter, the higher the welding temperature will be needed. Formation energies of X-shaped junctions have been systematically studied, which shows clearly a size effect. This size effect may be due to the strain energy of small nanotubes and the energy required for defect formation in SWNTs. For example, the formation energy of a Stone-Wales (SW) defect in SWNTs is a function of the diameter of SWNTs. This was demonstrated by a first principle calculation based on the extended Hückel method. The formation energy of SW defects was fitted to a simple formula as a function of the tube radius and the orientation of a SW defect in the tube, which provides a convenient tool for the study of thermodynamics and kinetics of SW defects in SWNTs. This work was partially supported by research grants from The Hong Kong Polytechnic University (A-PE54) and Research Grand Council of Hong Kong (PolyU 5306/03E).

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